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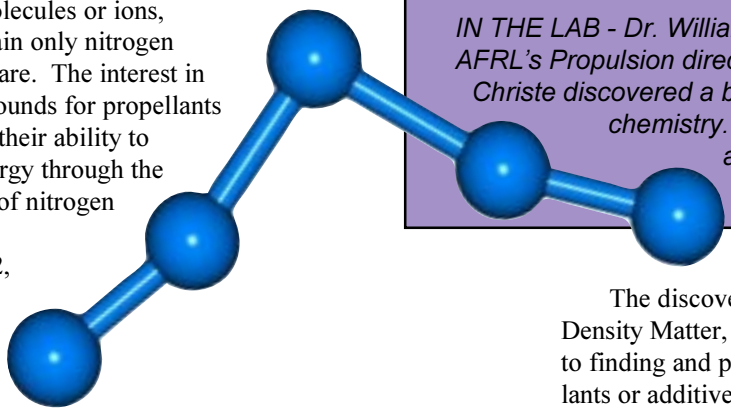
Chemists corner cation; propulsion use predicted

by Ranney Adams, Propulsion directorate

EDWARDS AFB, CALIF. - Researchers at the Air Force Research Laboratory have achieved a breakthrough in polyatomic nitrogen chemistry that may allow future advances in high-energy rocket propellants or explosives.

The new discovery, announced January 19 at the Winter Flourine Conference of the Division of Flourine Chemistry of the American Chemical Society, was made by Dr. Karl O. Christe and Dr. William W. Wilson of the AFRL Propulsion directorate. Led by Col. John R. Rogacki, the directorate is responsible for basic research, exploratory and advanced propulsion technology development.

Although nitrogen makes up 80 percent of the earth's atmosphere, polyatomic nitrogen molecules or ions, which contain only nitrogen atoms, are rare. The interest in these compounds for propellants stems from their ability to provide energy through the production of nitrogen molecules.



In 1772, notable chemists of the time, Rutherford, Sceele and Cavendish were able to isolate pure nitrogen from air. Only one polynitrogen compound, an azide anion, has ever been produce in bulk form. Curtius made this discovery in 1890.

The new discovery is a N_5^+ cation combined with the AsF_6^- anion, or $N_5^+AsF_6^-$. Christe devised the synthesis of the compound and Dr. Wilson was able to produce macroscopic amounts of the compound with high yield and purity. Considering the cation's calculated heat of formation of 353k cal/mol, the white solid compound is surprisingly stable.

Christe and his fellow researchers envision additional molecules with greater stability and potential for the future. For example, the new cation may be combined with an energetic anion to yield a highly energetic propellant or explosive ingredients.

IN THE LAB - Dr. William W. Wilson (pictured) of the AFRL's Propulsion directorate and his counterpart Karl O. Christe discovered a breakthrough in polyatomic nitrogen chemistry. Wilson produced macroscopic amounts of a new compound with high yield and purity.

The discoverers are part of the Lab's High Energy Density Matter, or HEDM, team. Their efforts are devoted to finding and producing new, high-powered rocket propellants or additives that exceed current capabilities for use in future Air Force systems. HEDM research at the lab is partially supported by Dr. Mike Berman of the Air Force Office of Scientific Research and by the Defense Advanced Research Project Agency.

Using the power of the world's largest computers, team members can predict the properties of exotic yet-to-be-made compounds while other scientists in the group make and test the new high-energy materials in the laboratory. Promising propellant candidates are then made in larger quantities and transitioned to the aerospace industry for additional evaluation.

Led by Dr. Pat Carrick, the Lab's HEDM team acted to validate and verify all aspects of the new molecule. Drs. Jerry Boatz, Jeffrey Sheehy and Mario Fajardo provided important theoretical and spectroscopic data from lab tests. This data agreed with information from Alan Kersham at the

THE DYNAMIC DUO - The new discovery was announced by Dr.Karl O. Christe (left) and Dr. William W. Wilson of the Propulsion directorate at the Winter Flourine Conference of the Division of Flourine Chemistry of the American Chemical Society on January 19.

University of Southern California and Dr. John Stanton at the University of Texas in Austin. Previous calculations made by Drs. Pyykkoe and Runeberg of the University of Helsinki, Finland, were also utilized.

The team also collaborated with the Loker Hydrocarbon Research Institute and Chemistry Department at the University of Southern California, where Christe guides a separate research group funded by the National Science Foundation. @